Munich Center for Machine Learning (MCML)
TUM School of Computation, Information and Technology
Technical University of Munich

Confidence in Causal Inference under Structure Uncertainty

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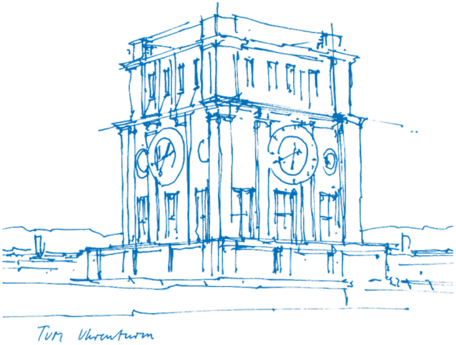

Starting point

- **Research question:** What is the total causal effect of X_i on X_j? Confidence?
- **Given:** Observational data in form of n samples of $(X_1, ..., X_d)$.
- **Problem:** Causal structure unknown.

Starting point

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- **Given:** Observational data in form of n samples of $(X_1, ..., X_d)$.
- **Problem:** Causal structure unknown.
- Naive two-step approach?
  (1) Learn causal structure.
  (2) Calculate confidence intervals for causal effects in inferred model.

Setup

Underlying Linear SCM with equal error variances

- **Example:**

$$
\begin{aligned}
X_1 &= \beta_{13} X_3 + \varepsilon_1 \\
X_2 &= \beta_{21} X_1 + \beta_{24} X_4 + \beta_{25} X_5 + \varepsilon_2 \\
X_3 &= \varepsilon_3 \\
X_4 &= \beta_{41} X_1 + \varepsilon_4 \\
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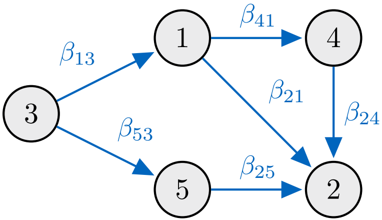
\end{aligned}
$$



where $\varepsilon_j \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$

Setup

Underlying Linear SCM with equal error variances

- **Example:** Causal effect $\mathcal{C}(1 \to 2) := \frac{\mathrm{d}}{\mathrm{d}x_1}\mathbb{E}[X_2 | \operatorname{do}(X_1 = x_1)] = \Sigma_{12|p(1)}/\Sigma_{11|p(1)}$.

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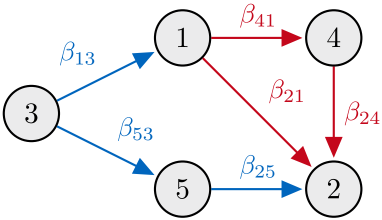

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Setup

- **Main Idea:** Use test inversion.

Tests for $\mathrm{H}_0^{(\psi)} : \mathcal{C}(i \to j) = \psi$ $\longrightarrow$ Confidence interval for $\mathcal{C}(i \to j)$

- **Goal:** Construct suitable **tests for all possible effects.**

Setup

- **Main Idea:** Use test inversion.

Tests for $\mathsf{H}_0^{(\psi)} : \mathcal{C}(i \to j) = \psi$	$\longrightarrow$	Confidence interval for $\mathcal{C}(i \to j)$

- **Goal:** Construct suitable **tests for all possible effects.**

- **Difficulty:** Each Hypothesis of fixed effect is **union of single hypotheses** over all DAGs on d nodes.

$$\mathsf{H}_0^{(\psi)} := \bigcup_{G \in \mathcal{G}(d)} \mathsf{H}_0^{(\psi)}(G)$$

Setup

- Linear SCM with equal error variances: $\mathcal{M} := \bigcup_{G \in \mathcal{G}(d)} \mathcal{M}(G)$, where

$$\mathcal{M}(G) = \left\{ \Sigma \in \mathsf{PD}(d) : \exists \sigma^2 > 0 \text{ with } \sigma^2 = \Sigma_{k,k|p(k)} \quad \forall\, k = 1, \ldots, d \right\}.$$

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- Hypothesis of fixed total causal effect: $\mathcal{M}_\psi := \bigcup_{G\in\mathcal{G}(d)} \mathcal{M}_\psi(G)$, where

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- **Task**: For all $\psi \in \mathbb{R}$ and $G \in \mathcal{G}(d)$ invert joint test of structure and effect size:

$$\mathrm{H}_0^{(\psi)}(G) : \Sigma \in \mathcal{M}_\psi(G) \quad \text{against} \quad \mathrm{H}_1 : \Sigma \in \mathcal{M} \setminus \mathcal{M}_\psi(G).$$

Maximum Likelihood Estimation

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- **Problem**: Maximizing the Gaussian likelihood

$$\frac{2}{n}\ell_n(\Sigma) = -\log\det(2\pi\Sigma) - \mathrm{tr}(\Sigma^{-1}\hat{\Sigma})$$

with $\Sigma \in \mathcal{M}_\psi(G)$ is equivalent to minimizing

$$\mathrm{tr}((I_d - B)^T(I_d - B)\hat{\Sigma}))$$

where $B \in \mathbb{R}^G$ represents the direct causal effects between variables.

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- Fixing total causal effects is complex **polynomial constraints** on direct effects, namely

$$(I_d - B)^{-1}_{j,i} = \psi.$$

Dual Maximum Likelihood Estimation

- **Solution**: Maximizing the Dual likelihood

$$\frac{2}{n}\ell_n^{dual}(\Sigma) := -\log\det(2\pi\Sigma^{-1}) - \mathrm{tr}(\Sigma\widehat{\Sigma}^{-1})$$

with $\Sigma \in \mathcal{M}_\psi(G)$ is equivalent to minimizing

$$\mathrm{tr}((I_d - B)^{-1}(I_d - B)^{-T}\hat{\Sigma})) = \mathrm{tr}((I_d - T)^T(I_d - T)\hat{\Sigma}))$$

where $T \in \mathbb{R}^{-G}$ represents the negative total causal effects between variables.

Dual Maximum Likelihood Estimation

- **Solution**: Maximizing the Dual likelihood

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  where $T \in \mathbb{R}^{-G}$ represents the negative total causal effects between variables.

- Fixed total effect constraint only pertains to one parameter, namely

$$T_{i,j} = -\psi$$

Main Result

- **Main steps**:

  (1) Intersection union test.

  (2) Stochastic upper bound by relaxing alternative.

  (3) Dual-LRT with conservative critical values from upper bound.

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  (1) Intersection union test.

  (2) Stochastic upper bound by relaxing alternative.

  (3) Dual-LRT with conservative critical values from upper bound.

- **Result:** Asymptotic $(1-\alpha)$-confidence set for causal effect $\mathcal{C}(i \to j)$ is

$$\{\psi \in \mathbb{R} : \min_{G \in \mathcal{G}(d)\,:\, i <_G j} \text{dual-}\lambda_n^{(\psi)}(G) \leq \chi^2_{d,1-\alpha}\} \cup \{0 : \min_{G \in \mathcal{G}(d)\,:\, j <_G i} \text{dual-}\lambda_n^{(0)}(G) \leq \chi^2_{d-1,1-\alpha}\}$$

Computation

- **Bottleneck:** Superexponential growth of possible causal structures with nodes.

Computation

- **Bottleneck:** Superexponential growth of possible causal structures with nodes.
- 'Only' need to consider complete DAGs: d factorial structures.
- Branch and bound type search algorithm through causal orderings. Feasible up to 12 involved variables (already uncertainty over more than 10^{26} structures).

Conclusion

- Closed-form solution for constructing confidence regions for total causal effects that:
  - account for **causal structure uncertainty**
  - as well as **statistical uncertainty** about the numerical size of the effect.
- Conceptual ideas of leveraging test inversions of joint tests for causal structure and effect size generalizable to other modeling assumptions.
- Matrix inversion interplay between direct and total effects that is behind the use of dual likelihood can be exploited in other causal inference tasks.

Thank you!

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- Our related papers:
  - Strieder and Drton (2024). *Dual Likelihood for Causal Inference under Structure Uncertainty*. CLeaR 24. Preprint at arXiv.
  - Strieder and Drton (2023). *Confidence in Causal Inference under Structure Uncertainty in Linear Causal Models with Equal Variances*. J. Causal Inference 11 (1).
  - Strieder, Freidling, Haffner and Drton (2021). *Confidence in Causal Discovery with Linear Causal Models*. UAI 21.